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Dr. Richard S. Miller

Technical Report No. 97

COMPUTED HEATS OF FORMATION OF THREE TETRAAZAPENTALENES, A
TRIS(NITROTRIAZOLO)TRIAZINE, AND A TRICYCLIC *GEM*-
DIFLUORAMINO/TETRANITRAMINE

by

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November 14, 1996

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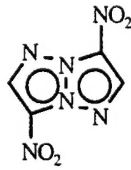
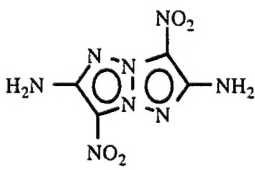
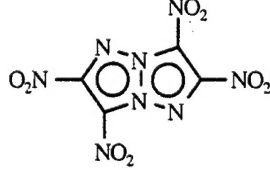
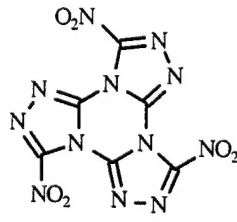
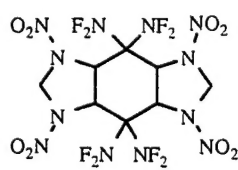
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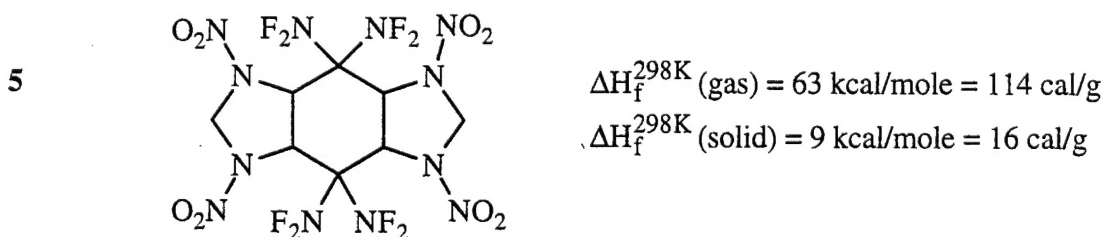
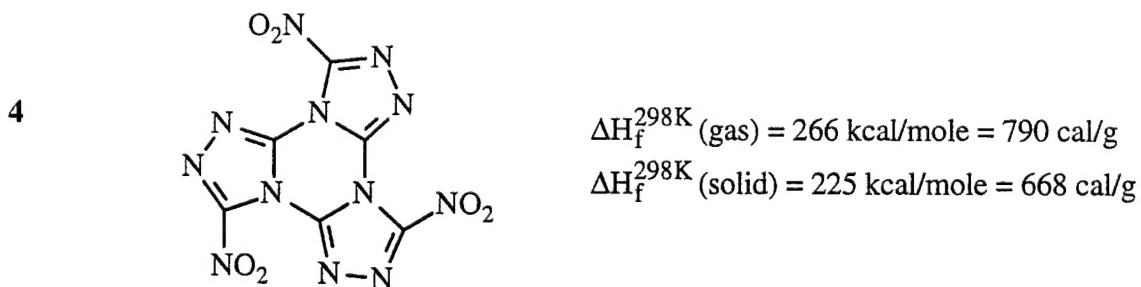
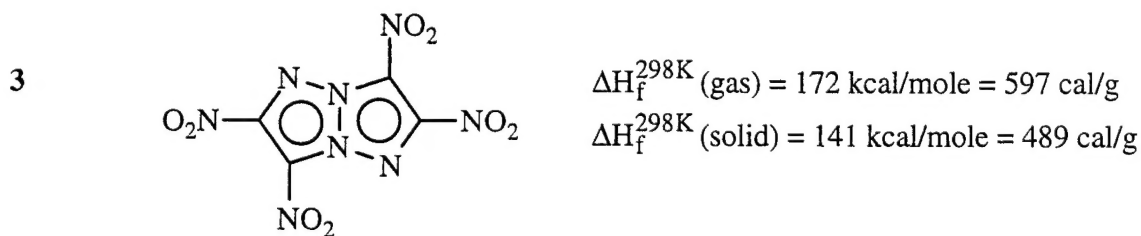
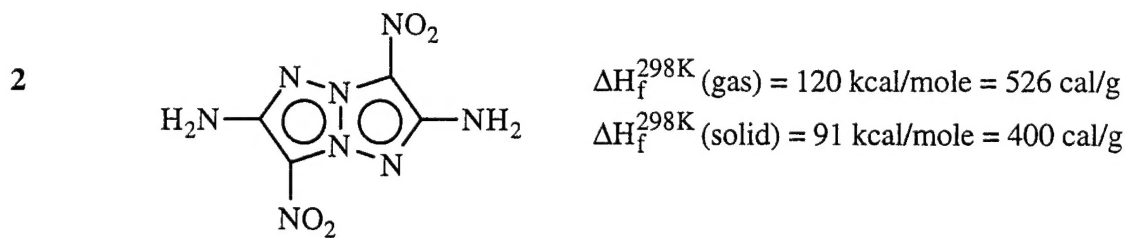
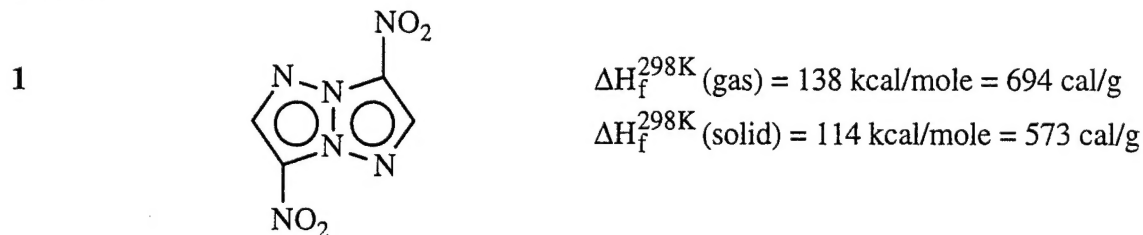
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| <div style="display: flex; justify-content: space-around; align-items: flex-end;"><div style="text-align: center;"> 1</div><div style="text-align: center;"> 2</div><div style="text-align: center;"> 3</div><div style="text-align: center;"> 4</div><div style="text-align: center;"> 5</div></div> | | | | |
| 1: ΔH_f^{298K} (solid) = 114 kcal/mole = 573 cal/g 4: ΔH_f^{298K} (solid) = 225 kcal/mole = 668 cal/g 2: ΔH_f^{298K} (solid) = 91 kcal/mole = 400 cal/g 5: ΔH_f^{298K} (solid) = 9 kcal/mole = 16 cal/g 3: ΔH_f^{298K} (solid) = 141 kcal/mole = 489 cal/g | | | | |
| 14. SUBJECT TERMS heats of formation; tetraazapentalenes; tris(nitrotriazolo)- triazine; tricyclic <u>gem</u> -difluoramino/tetranitramine | | | 15. NUMBER OF PAGES 4 | |
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We have used our density functional procedure [1] to compute the heats of formation of the compounds **1** - **5**, proposed by W. Koppes and A. Stern (ONR). The vibrational energies were determined from the molecular stoichiometries [2]. The density functional calculations give the gas phase heat of formation, which we convert to the solid state value by subtracting the heat-of sublimation. The latter is obtained by means of the relationship that we have developed between the heat of sublimation and the computed electrostatic potential on the molecular surface [3].

Results:



For comparison, the experimental gas phase ΔH_f^{298K} value for RDX is 206 cal/g [4,5].

References:

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